

Gluconolactone  
90-80-2 | DTXSID0026549

Model Performance

|       |      |
|-------|------|
| Model | Data |
|-------|------|

Weighted KNN model

| 5-fold CV (75%) |      | Training (75%) |      | Test (25%) |      |
|-----------------|------|----------------|------|------------|------|
| Q2              | RMSE | R2             | RMSE | R2         | RMSE |
| 0.85            | 1.14 | 0.85           | 1.12 | 0.83       | 1.23 |

## Model Results

**Predicted value:**  $8.08 \times 10^{-12}$  cm<sup>3</sup>/molecule\*sec

**Global applicability domain:** Inside

**Local applicability domain index:**  $3.39 \times 10^{-1}$

**Confidence level:**  $8.17 \times 10^{-1}$

## Nearest Neighbors from the Training Set

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Ethyl lactate

**Measured:**  $3.90 \times 10^{-12}$

**Predicted:**  $4.80 \times 10^{-12}$

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Methyl 2-hydroxypropanoate

**Measured:**  $2.80 \times 10^{-12}$

**Predicted:**  $3.16 \times 10^{-12}$

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2-Ethoxyethyl isobutyrate

**Measured:**  $1.35 \times 10^{-11}$

**Predicted:**  $1.28 \times 10^{-11}$

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Ethyl 3-ethoxypropionate

**Measured:**  $2.29 \times 10^{-11}$

**Predicted:**  $1.63 \times 10^{-11}$

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2-Ethoxyethyl acetate

**Measured:**  $1.30 \times 10^{-11}$

**Predicted:**  $1.03 \times 10^{-11}$